

Figure S1 Comparison of the predicted and true content of the samples.  $X$  denotes the raw dataset, while  $X_{PCA}$  and  $X_{SPCA}$  denote the datasets denoised using PCA and SPCA, respectively. The insets show the prediction errors' histogram. The blue line represents perfect prediction.

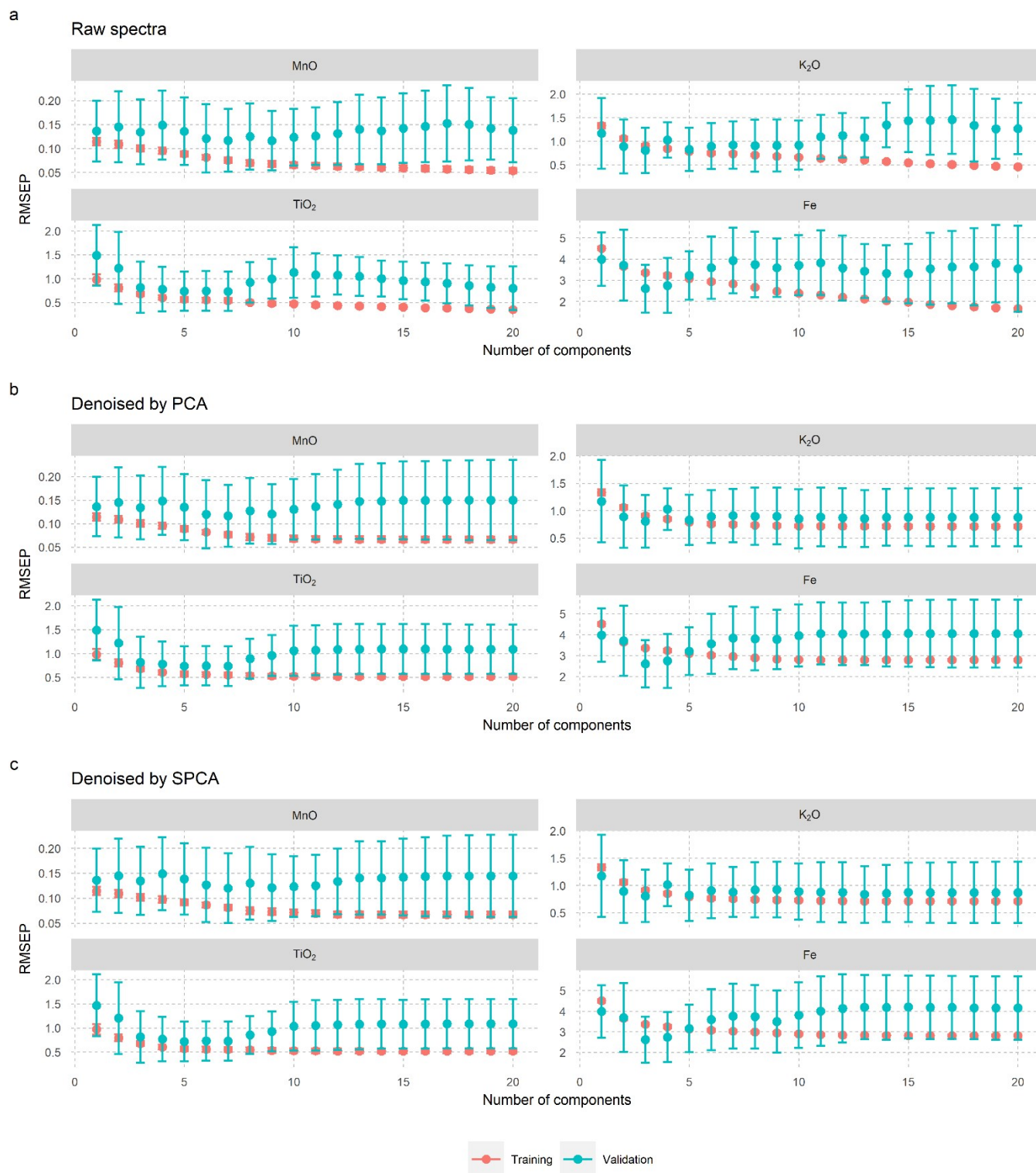


Figure S2 RMSEP results from the 10-fold cross validation for the PLS models. The error bars represent the standard deviation.

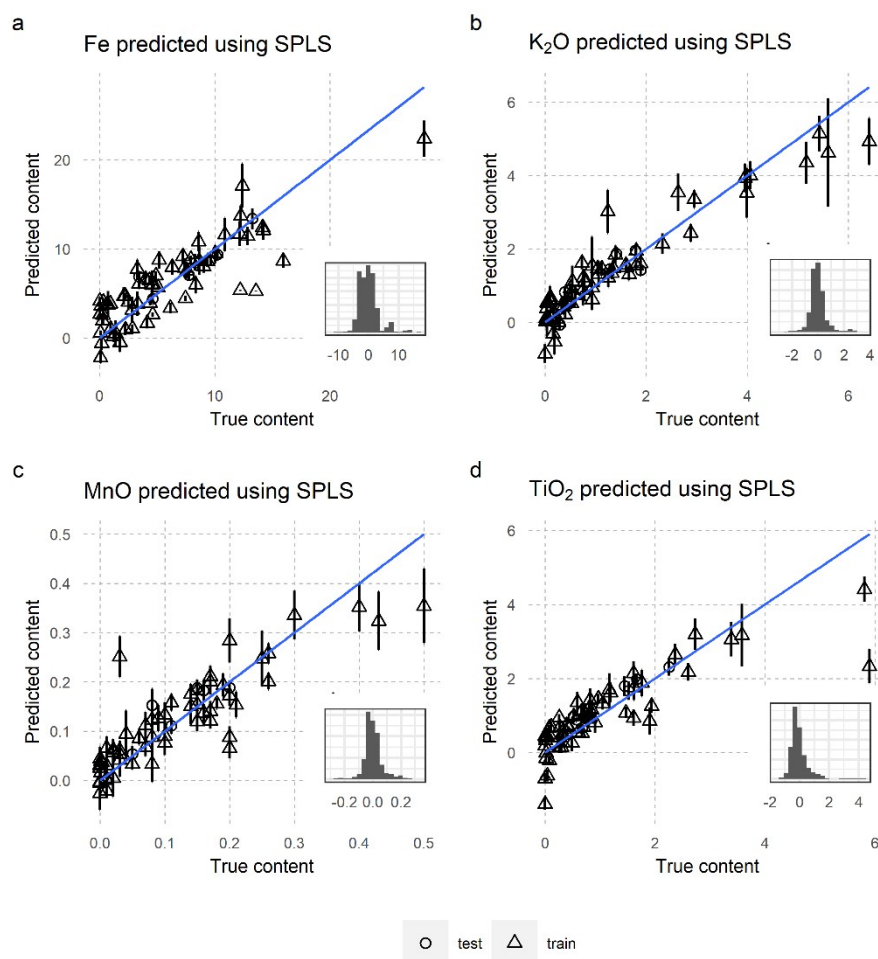


Figure S3 Comparison of the predicted and true content of the samples. The insets show the prediction errors' histogram. The blue line represents perfect prediction.

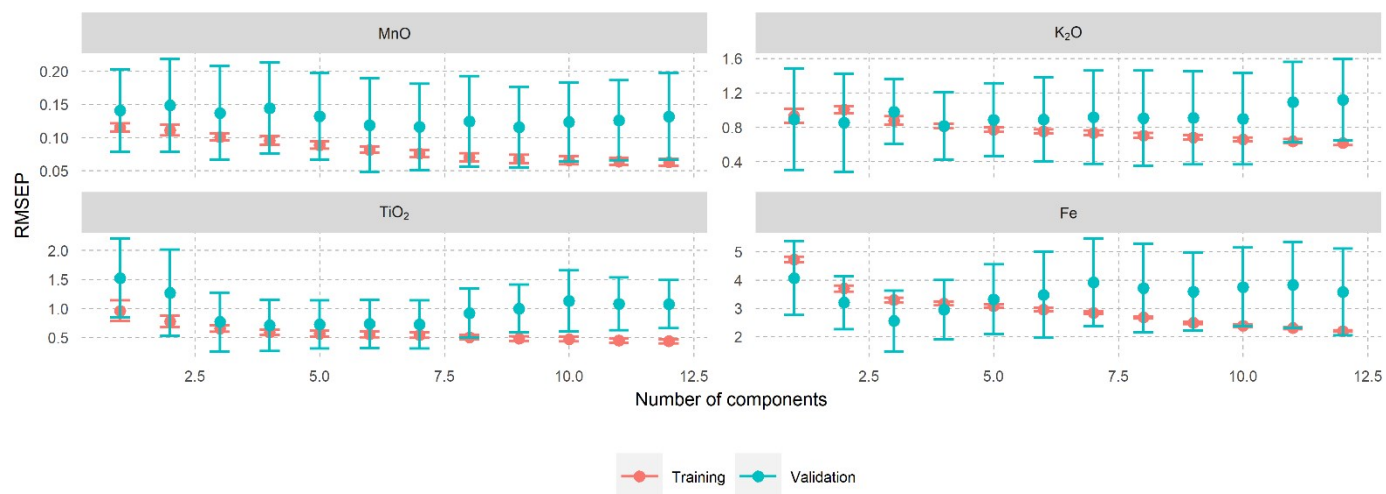


Figure S4 RMSEP results from the 10-fold cross validation for the SPLS models. The error bars represent the standard deviation.